TECHNICAL REPORT CR-RD-PR-89-1

FURTHER INVESTIGATION OF FLOW MODELING DURING SOLID PROPELLANT PROCESSING

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MAY 1989

Prepared for:
Propulsion Directorate
Research, Development, and Engineering Center

Contract No. W-31-109-ENG-38

U.S. ARMY MISSILE COMMAND
Redstone Arsenal, Alabama 35898-5000

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by

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UNCLASSIFIED
SECURITY CLASSIFICATION OF THIS PAGE

REPORT DOCUMENTATION PAGE

Form Approved
OMB No 0704-0188
Exp Date Jun 30, 1986

1a REPORT SECURITY CLASSIFICATION: Unclassified

1b. RESTRICTIVE MARKINGS:

2a SECURITY CLASSIFICATION AUTHORITY:

2b. DECLASSIFICATION / DOWNGRADING SCHEDULE:

3. DISTRIBUTION / AVAILABILITY OF REPORT: Approved for public release, distribution is unlimited.

4. PERFORMING ORGANIZATION REPORT NUMBER(S):

5. MONITORING ORGANIZATION REPORT NUMBER(S): CR-RD-PR-89-1

6a NAME OF PERFORMING ORGANIZATION: Argonne National Laboratory Components Technology Div

6b. OFFICE SYMBOL (If applicable):

7a. NAME OF MONITORING ORGANIZATION: Propulsion Directorate, Research, Development and Engineering Center

6c. ADDRESS (City, State, and ZIP Code): 9700 South Cass Avenue Argonne, IL 60439

7b. ADDRESS (City, State, and ZIP Code): Commander U.S. Army Missile Command ATTN: AMSMI-RD-PR Redstone Arsenal, AL 35898-5249

8a. NAME OF FUNDING / SPONSORING ORGANIZATION: Propulsion Directorate, Res. Dev. and Eng Ctr

8b. OFFICE SYMBOL (If applicable): AMSMI-RD-PR-E

9. PROCUREMENT INSTRUMENT IDENTIFICATION NUMBER: Contract No. W-31-109-ENG-38

8c. ADDRESS (City, State, and ZIP Code): Commander U.S. Army Missile Command ATTN: AMSMI-RD-PR Redstone Arsenal, AL 35898-5249

10. SOURCE OF FUNDING NUMBERS

PROGRAM ELEMENT NO.	PROJECT NO.	TASK NO.	WORK UNIT ACCESSION NO
61101A	IL161101A91A		

11. TITLE (Include Security Classification): Further Investigation of Flow Modeling During Solid Propellant Processing (U)

12. PERSONAL AUTHOR(S): Y. S. Cha, H. M. Domanus, W. T. Sha, S. L. Soo

13a. TYPE OF REPORT	13b. TIME COVERED	14. DATE OF REPORT (Year, Month, Day)	15. PAGE COUNT
Final	FROM 9/87 TO 9/88	May 1989	35

16. SUPPLEMENTARY NOTATION:

17. COSATI CODES			18. SUBJECT TERMS (Continue on reverse if necessary and identify by block number)
FIELD	GROUP	SUB-GROUP	Propellant Processing Flow Modeling Liquid/Solid Flows
21	08		

19. ABSTRACT (Continue on reverse if necessary and identify by block number)

A two-fluid model is employed to investigate the velocity and volume fraction distributions during the solid propellant casting process. Two important dimensionless parameters, the dimensionless interfacial momentum transfer coefficient D, and the viscosity ratio of the two fluids Z, are identified and varied parametrically in the numerical calculations. The results show that when D is small (< 0.05), separation between the particles and binder occurred and the smaller the D, the larger the degree of separation. When D is large (> 1), separation did not occur since the two fluids move like a single fluid when interfacial momentum transfer is dominating. Near the transition point between separation and no separation (D ≅ 1), an M-shaped profile was observed for the particle volume fraction distribution in an annular duct. The degree of separation is very small and the reason for the existence of such an M-shaped profile is not clearly understood.

(Continued)

20. DISTRIBUTION / AVAILABILITY OF ABSTRACT: ☒ UNCLASSIFIED/UNLIMITED ☐ SAME AS RPT. ☐ DTIC USERS

21. ABSTRACT SECURITY CLASSIFICATION: Unclassified

22a. NAME OF RESPONSIBLE INDIVIDUAL: A. R. Maykut

22b TELEPHONE (Include Area Code): (205)876-0075

22c. OFFICE SYMBOL: AMSMI-RD-PR

DD FORM 1473, 84 MAR — 83 APR edition may be used until exhausted. All other editions are obsolete.

Block 19. (Continued)

It is pointed out that a viscosity model recently proposed by Probstein and Sengun may be relevant to the solid propellant system. It is suggested that the next logical step is to incorporate the non-Newtonian behavior of the binder (and the fine particles) into the two-fluid model.

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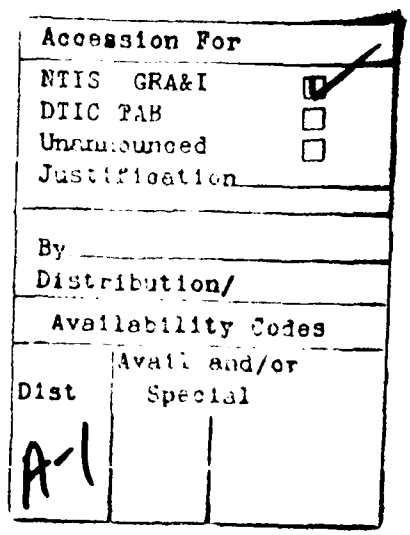

1.0. INTRODUCTION

It was observed that a bump existed in the pressure-time curve during the burning of solid rocket propellant. The pressure bump is likely due to a concentration of ammonium perchlorate in the propellant, and thus related to the filling process [1]. A common feature of all propellant compositions giving a bump is a high solids fraction, not less than 70% by weight (mostly ammonium perchlorate) dispersed in a binder. Unfortunately, the current understanding of a densely packed particle/fluid system is rather poor and no simple explanation is satisfactory. Furthermore, non-Newtonian behavior is expected during the filling process which makes the theoretical analysis of the practical system very difficult.

In a previous report [2], preliminary investigation was performed by using the multiple velocity field model. This is a continuum approach as opposed to a discrete particle track. It was demonstrated in the preliminary investigation that, by using different velocity boundary conditions for the two fluids, partial component separation was predicted. No slip was assumed for the liquid binder while free slip was assumed for the ammonium perchlorate particles, since particle velocity may have a finite value at the wall. Even though the results are encouraging, it was pointed out that while the multifluid model is more complete than the diffusion model, there are more unknown coefficients associated with the model, and these coefficients need to be determined either experimentally and/or theoretically.

In this report, the multifluid model will be adopted. Emphasis will be placed on identifying important parameters (dimensional or dimensionless) for the two-fluid model. An attempt will be made to narrow down the parameters range and to interpret the results of the multifluid model that are relevant to the solid propellant casting process.

2.0. IMPORTANT PARAMETERS

The momentum equations for a two-fluid system are

$$\frac{\partial}{\partial t}(\theta_1\rho_1\bar{U}_1) + \nabla\cdot(\theta_1\rho_1\bar{U}_1\bar{U}_1)$$

$$= -\theta_1\nabla P + \nabla\cdot\bar{\bar{\tau}}_{1m} + \theta_1\rho_1\bar{f}_1 - K_{12}(\bar{U}_1 - \bar{U}_2) \qquad (1)$$

$$\frac{\partial}{\partial t}(\theta_2\rho_2\bar{U}_2) + \nabla\cdot(\theta_2\rho_2\bar{U}_2\bar{U}_2)$$

$$= -\theta_2\nabla P + \nabla\cdot\bar{\bar{\tau}}_{2m} + \theta_2\rho_2\bar{f}_2 - K_{21}(\bar{U}_2 - \bar{U}_1) \qquad (2)$$

where θ_1, ρ_1, $\bar{U}_1$ refer to the volume fraction, the material density, and the velocity of the binder respectively, subscript 2 refers to the particles (ammonium perchlorate), τ_{1m} is the shear stress of component 1 in the mixture, f_1 is the field force per unit mass on component 1 and may include that due to shear lifting effect, P is pressure, K_{12} is the interfacial momentum transfer

coefficient between the two phases, etc. The parameters and properties needed are f_1, f_2, τ_{1m}, τ_{2m}, θ_1, θ_2, f_1, f_2, K_{12}, and K_{21}. Additonal key parameters are the particle size and its distribution. The volume fractions are related,

$$\theta_1 + \theta_2 = 1 \tag{3}$$

The field forces (f_1 and f_2) will be treated separately and are not included in the present investigation. The shear stress terms (τ_{1m} and τ_{2m}) are not readily determined at this time for dense suspensions. In the numerical calculations, it is simply assumed that each of the two fluids behave in a Newtonian fashion and the viscosity of each fluid is not affected by the presence of the other fluid. Even with this simplified assumption, it is still difficult to determine the viscosity of the second fluid, i.e., ammonium perchlorate particles.

The interfacial momentum transfer coefficients (K_{12} and K_{21}) can be expressed as

$$K_{12} = \theta_1 \rho_1 F_{12} , \tag{4}$$

$$K_{21} = \theta_2 \rho_2 F_{21} , \tag{5}$$

where F_{12} is the inverse relaxation time for momentum transfer from phase 2 to phase 1, etc., and

$$K_{12} = K_{21} \tag{6}$$

from action and reaction. For the motion of a particle suspended in a fluid in the Stokes regime [3],

$$F_{21} = \frac{9\mu_1}{2\, a^2\, \rho_2} , \tag{7}$$

where a is the radius of the particle, μ_1 is the viscosity of the fluid, and ρ_2 is the material density of the particle. Combining Eqs. 5, 6, and 7, the following equation is obtained:

$$\frac{K_{12}\, a^2}{\mu_1} = \frac{9\, \theta_2}{2} . \tag{8}$$

If a dimensionless interfacial momentum transfer coefficient is defined as

$$D = \frac{K_{12}\, a^2}{\mu_1} , \tag{9}$$

then

$$D = \frac{9\,\theta_2}{2}\,, \tag{10}$$

which is valid only for a single particle suspended in a fluid medium in the Stoke's regime.

For a cloud of particles suspended in a fluid stream, the inverse relaxation time is [3],

$$F_{21} = \frac{75\,(1-\theta_1)\,\mu_1}{2\,\theta_1^2\,\rho_2\,a^2} + \frac{1.75\,\rho_1 u_s}{2\,\theta_1^2\,\rho_2\,a} \tag{11}$$

where u_s is the superficial fluid velocity based on unobstructed flow area. In the interest of the solid propellant system, the largest particle size is in the order of a = 100 μm. The viscosity of the binder (μ_1) is relatively large (~200 Pa-s versus 10^{-3} Pa-s for room temperature water). Thus, the first term on the right-hand side is dominating for the solid propellant system. Therefore, Eq. 11 can be written

$$F_{21} \cong \frac{75\,\theta_2\,\mu_1}{2\,\theta_1^2\,\rho_2\,a^2}\,. \tag{12}$$

Combining Eqs. 4, 5, and 12,

$$D = \frac{K_{12}\,a^2}{\mu_1} = \frac{75}{2}\left(\frac{\theta_2}{\theta_1}\right)^2\,. \tag{13}$$

Equations 10 and 13 indicate that the dimensionless interfacial momentum transfer coefficient, which is a function of volume fraction only, is the relevant scaling parameter for interfacial momentum transfer. For given volume fraction (θ_1 or θ_2), Eqs. 10 and 13 can be used to estimate the order of magnitude of D for single particle and a cloud of particles suspended in a fluid stream, respectively.

In addition to the dimensionless interfacial momentum transfer coefficient D, the viscosity ratio, defined as

$$Z = \frac{\mu_2}{\mu_1}\,, \tag{14}$$

is another important parameter since the velocity and volume fraction distributions will depend strongly on the relative magnitude of the two viscosities in the two-fluid model.

The particle size and its distribution will significantly affect the outcome of the solid propellant casting process. The two-fluid model is not capable of dealing with a system with a number of particle sizes. However, by using certain physical models, such as the Probstein-Sengun bimodal model [4],

it is possible to include the contribution from various particle sizes in a two-fluid model, and therefore avoid going to a multifluid model which will only introduce more unknowns, with current status of knowledge a fluid system with multiple particle sizes.

3.0. EFFECTS OF INTERFACIAL DRAG AND RELATIVE VISCOSITY

To investigate the effects of interfacial momentum transfer and relative viscosity of two fluids, steady-state calculations were performed for an annular flow, which is the two-dimensional axisymmetric flow between two concentric cylindrical surfaces employed in previous investigations [2]. The characteristics of the geometry, values of properties, and boundary conditions are given in Table 1.

Table 1. Properties and Characteristics of Annular Flow

Inner Radius, R_i	1.905 cm
Outer Radius, R_o	2.540 cm
Gap	0.635 cm
Inlet Velocity $U_1 = U_2 = U_o$	1.0 cm/s
Inlet Volume Fraction	
θ_1 (binder)	0.2242
θ_2 (particle)	0.7758
Material density	
ρ_1 (binder)	920 kg/m^3
ρ_2 (particle)	1950 kg/m^3
Velocity Boundary Condition	
Binder	no slip
Particle	free slip

An average particle size with a radius of 100 μm is assumed. Since the average diameter (or radius) is used, the particle volume fraction can exceed the maximum packing fraction for particles with a single diameter. The binder viscosity (μ_1) is assumed to be equal to 200 Pa-s.

Figures 1 through 8 show the fully-developed velocity and volume fraction distributions at the exit of an annular duct for different values of the dimensionless interfacial momentum transfer coefficient D, and viscosity ratio Z. For a viscosity ratio of Z = 1, Figs. 1 through 4 indicate that the effects of interfacial parameter D begin to appear when it is decreased from 0.50 to 0.05 and the effects become appreciable when D = 0.005. Significant separation occurred when D = 0.005, as shown in Figs. 3 and 4. When the interfacial momentum transfer coefficient is large ($D \geq 0.5$), there is very

little separation and the volume fraction of either the binder or the particle remains nearly constant across the duct. This is understandable since the two fluids will move as a single fluid if the interfacial drag D becomes large.

Figures 5 through 8 show the effects of viscosity ratio ($Z = \mu_2/\mu_1$) on velocity and volume fraction distributions for D = 0.005. It can be observed that the viscosity ratio affects the volume fraction distribution somewhat, but the most pronounced effect appears in the particle velocity distribution as shown in Fig. 6. If the particle viscosity is much larger than the binder viscosity (for example, Z = 8.70), then the particles move in a manner as if the binder is absent. On the other hand, if the binder viscosity is much larger than that of the particles (for example, Z = 0.04), the particle velocity distribution becomes closer to the binder velocity distribution. The binder velocity distribution appears to be less sensitive to the viscosity ratio.

Two additional interesting phenomena were observed from the numerical results. If the interfacial momentum transfer coefficient is large (D > 1), the volume fraction distributions for both the binder and the particles are uniform and are independent of the value of the viscosity ratio Z. This means that there is a limiting value of D ($\cong$1), above which there is no separation and below which separation does occur. This result indicates that it is extremely important to determine the value of the dimensionless interfacial momentum transfer coefficient for the solid propellant system. The authors are not aware of any existing theoretical/experimental model that can accurately predict the value of D for a densely packed system such as the solid propellant system. Further experimental and theoretical investigation in this direction will be very helpful.

The second interesting phenomenon occurs near the transition point between separation and no separation (D $\cong$ 1). Figures 9 and 10 show the binder and the particle volume fraction distributions for D = 1 and Z = 10. At such a high value of D, separation is minute, but finite. This can be observed from the M-shaped or W-shaped profile and the small increment in the vertical scale shown in Fig. 9 or 10. The reason for the existence of an M-shaped (or W-shaped) profile is not clearly understood at this time.

4.0. DISCUSSIONS

In the preliminary investigation, both the multifluid model and the single velocity field model were proposed [2]. In the multifluid model, the transport properties F_{12}, μ_m, etc., are not readily computed or measured. The closeness of the phase velocities suggest that the mixture velocity may be sufficiently representative. This leads to the development of a single velocity field model described in Ref. 2. It is recognized that the inverse relaxation time (F_{12}) and the mixture viscosity μ_m still have to be determined experimentally. However, it is difficult to visualize how a single fluid model can produce particle separation observed in the solid propellant system.

In the investigation of dense slurry rheology, Probstein and Sengun [4] recently proposed a bimodal model to describe the polymodal behavior of coal-water slurries. Their model appears to have some merit and seems relevant to the solid propellant casting process. In the bimodal model, the following definitions were employed

$$\theta_v = \frac{V_c + V_f}{V_c + V_f + V_\ell}$$

$$\theta_{ff} = \frac{V_f}{V_f + V_\ell}$$

$$\theta_c = \frac{V_c}{V_f + V_\ell + V_c}$$

where θ_v is the volume fraction of the suspended solids, θ_{ff} is the fine-filler volume fraction, θ_c is the coarse particle volume fraction, V_f is the volume of the fine filler, V_c is the volume of the coarse particles, and V_ℓ is the volume of the fluid. It is further defined that

$$\eta_{nr} = \eta_{cr} \cdot \eta_{fr} = \left(\frac{\mu_c}{\mu_f}\right)\left(\frac{\mu_f}{\mu_o}\right)$$

where

η_{nr} = net relative viscosity = μ_c/μ_o,

η_{cr} = coarse relative viscosity = μ_c/μ_f,

η_{fr} = fine relative viscosity = μ_f/μ_o,

μ_c = apparent viscosity of the suspension,

μ_f = apparent viscosity the suspending fluid with fine particles present, and

μ_o = viscosity of the pure liquid.

The basic assumptions in the Probstein-Sengun model are

$$\eta_{cr} = f(\theta_c)$$

and

$$\eta_{fr} = f(\theta_{ff}).$$

They further assumed that it is the small volume fraction of the colloidal size particles that imparts to the suspension most of its rheological characteristics (shear rate dependent viscosity). The large particles are essentially unaware of the presence of fine particles, but rather see a stiffened fluid that has the same viscosity and density as the suspension, with the contribution of the large particles to the viscosity increase coming about from hydrodynamic dissipation (independent of shear rate). These assumptions were supported by experimental data at low shear rate. The demarkation between fine and coarse volume fractions for six different coal/water slurries ranged from 2 to 8 microns, with an average of about 4.5 microns, even though the particle diameters in the slurries ranged from 0.5 to 300 microns. Thus, the viscosity of a polymodal system can be represented approximately by the viscosity of a bimodal system. This greatly simplifies the analysis and therefore is the more practical approach than the multifluid

model. The composition of solid propellant contains particles and powders of various sizes and is extremely difficult to handle. The bimodal model of Probstein and Sengun appears to offer a reasonable alternative. Of course, there are limitations for the application of the bimodal model as described in Ref. 4. In addition, the bimodal model does not address the problems related to particle/particle interaction, shear lift, and particle/ wall interaction.

5.0. SUMMARY

(1) A two-fluid model is employed to investigate the velocity and volume fraction distributions in an annular duct. A no slip boundary condition was assumed for the fluid (the continuous phase) and free slip was assumed for the particles (the dispersed phase) at the walls. Two important dimensionless parameters were identifed and parametric studies were carried out by varying these parameters. The most important parameter is the dimensionless interfacial momentum transfer coefficient D $(= K_{12}a^2/\mu_1)$, and the second parameter is the viscosity ratio of the two-fluid Z $(= \mu_2/\mu_1)$. Both parameters can affect the velocity and volume fraction distributions significantly.

(2) Numerical results indicate that for relatively small values of D, the dimensionless interfacial momentum transfer coefficient ($D < 0.05$), significant separation between the binder and the particles are observed. The smaller the D, the larger the degree of separation. Viscosity ratio Z also affects the volume fraction distribution, but its influence is somewhat less than that of the interfacial momentum transfer coefficient D.

(3) The degree of separation decreases with increasing values of the interfacial momentum transfer coefficient. When D is sufficiently high (>1), separation no longer exists. This is understandable since when interfacial momentum transfer is dominating, the two fluids move like a single fluid and consequently, there is very little separation. Currently, there is no theoretical or experimental model that can accurately predict the value of the interfacial momentum transfer coefficient for the solid propellant system. Further investigation, either theoretical or experimenhtal, in this direction will be extremely helpful.

(4) An interesting phenomenon is observed near the transition between separation and no separation ($D \cong 1$). The degree of separation is rather small at $D = 1$, but the particle volume fraction distribution exhibited an M-shaped profile which is not present for D much smaller than 1. The reason for the existence of such an M-shaped profile is not clearly understood at this time.

(5) The bimodal model proposed by Probstein and Sengun may be advantageous and relevant to the solid propellant system since it allows the use of a bimodal viscosity model to represent a polymodal system. This is a more practical approach than using the multifluid model since the latter will only introduce more unknowns.

(6) It is suggested that a logical next step is to incorporate the non-Newtonian behavior of the binder into the two-velocity numerical model. This can be accomplished by modifying the present computer program to include the effects of shear-rate dependent viscosity in the following form

$$u = c\left|\frac{\partial u}{\partial r}\right|^n,$$

where c is an empirical constant, $\frac{\partial u}{\partial r}$ is the local shear rate, and the exponent n accounts for various rheological behaviors of the fluid.

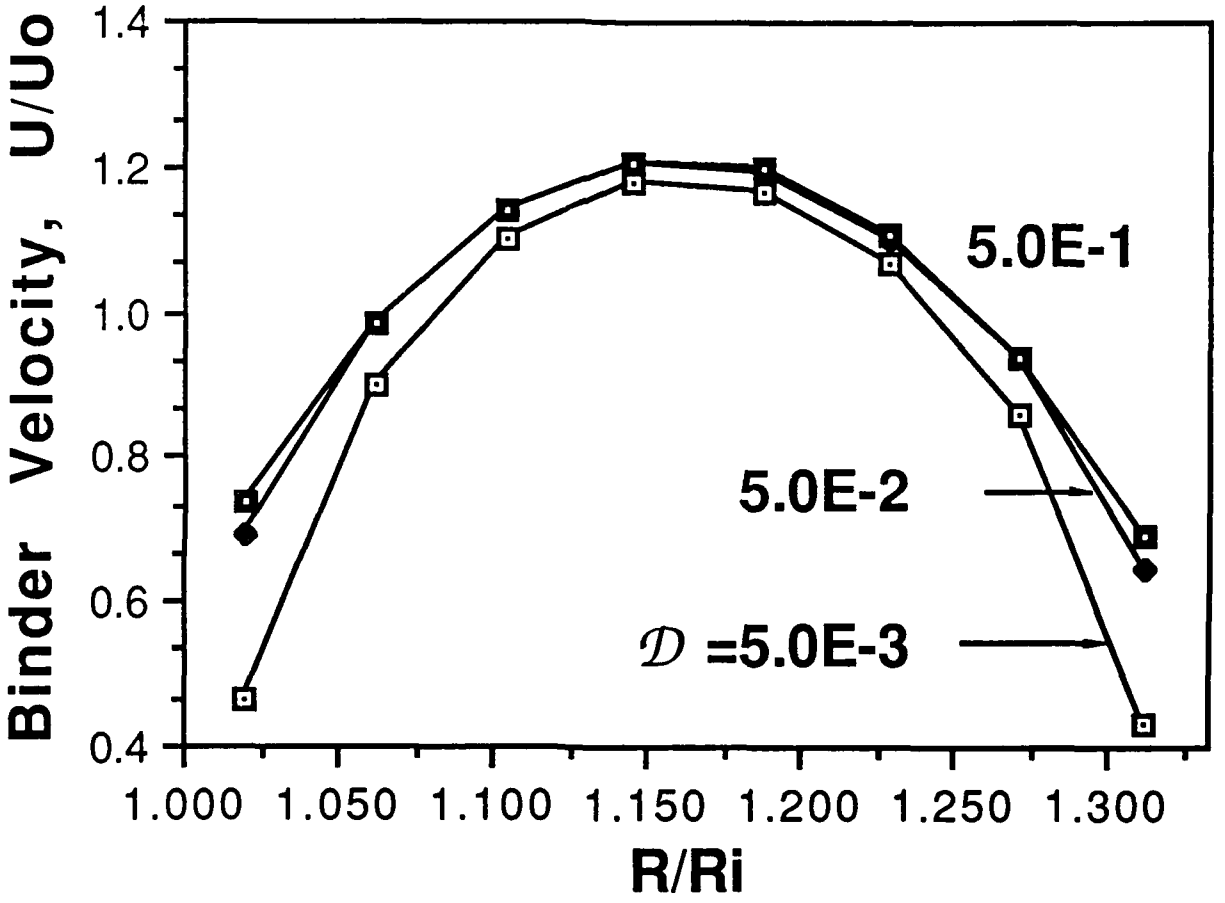

Fig. 1. Fully-Developed Velocity Distributions at the Exit of an Annular Duct (Z = 1)

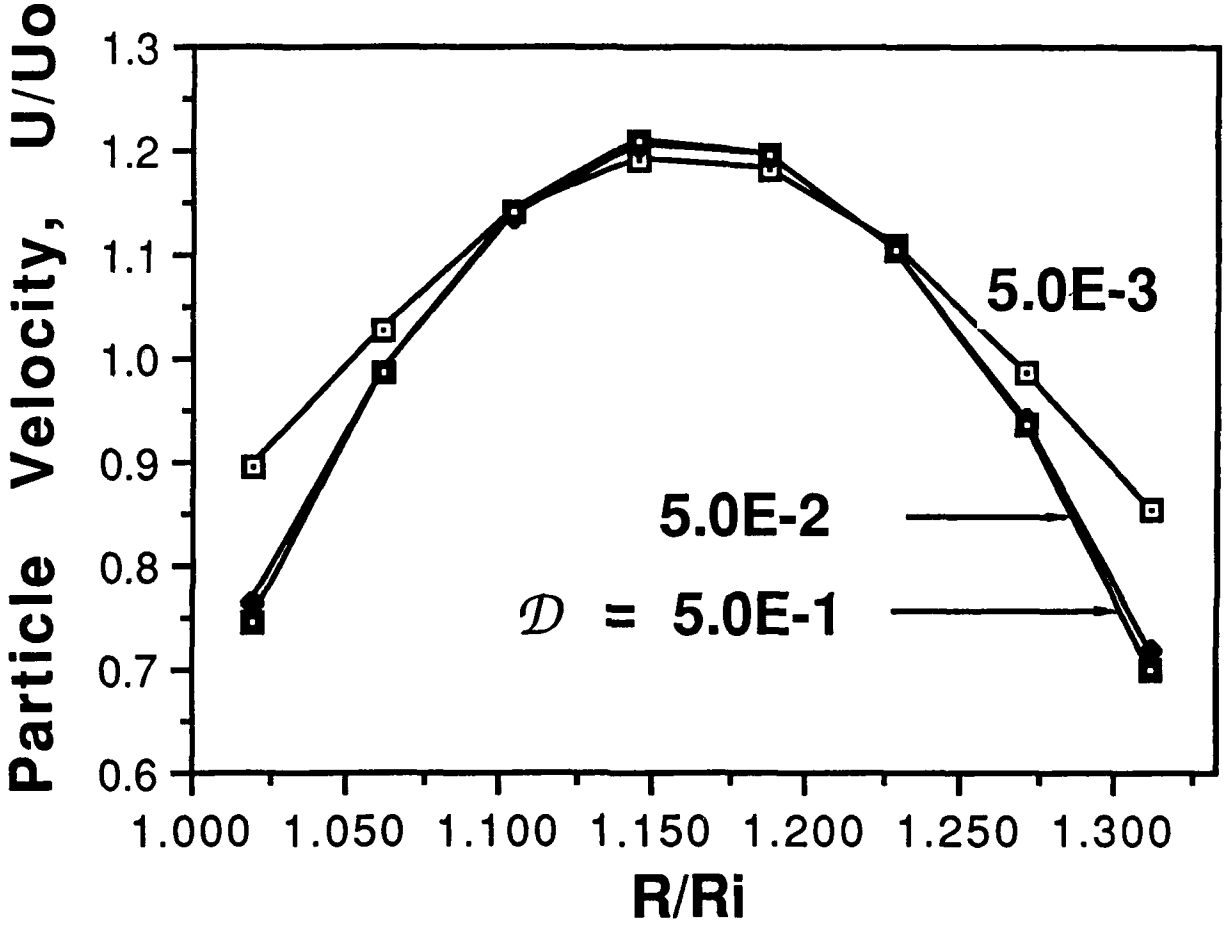

Fig. 2. Fully-Developed Particle Velocity Distribution at the Exit of an Annular Duct (Z = 1)

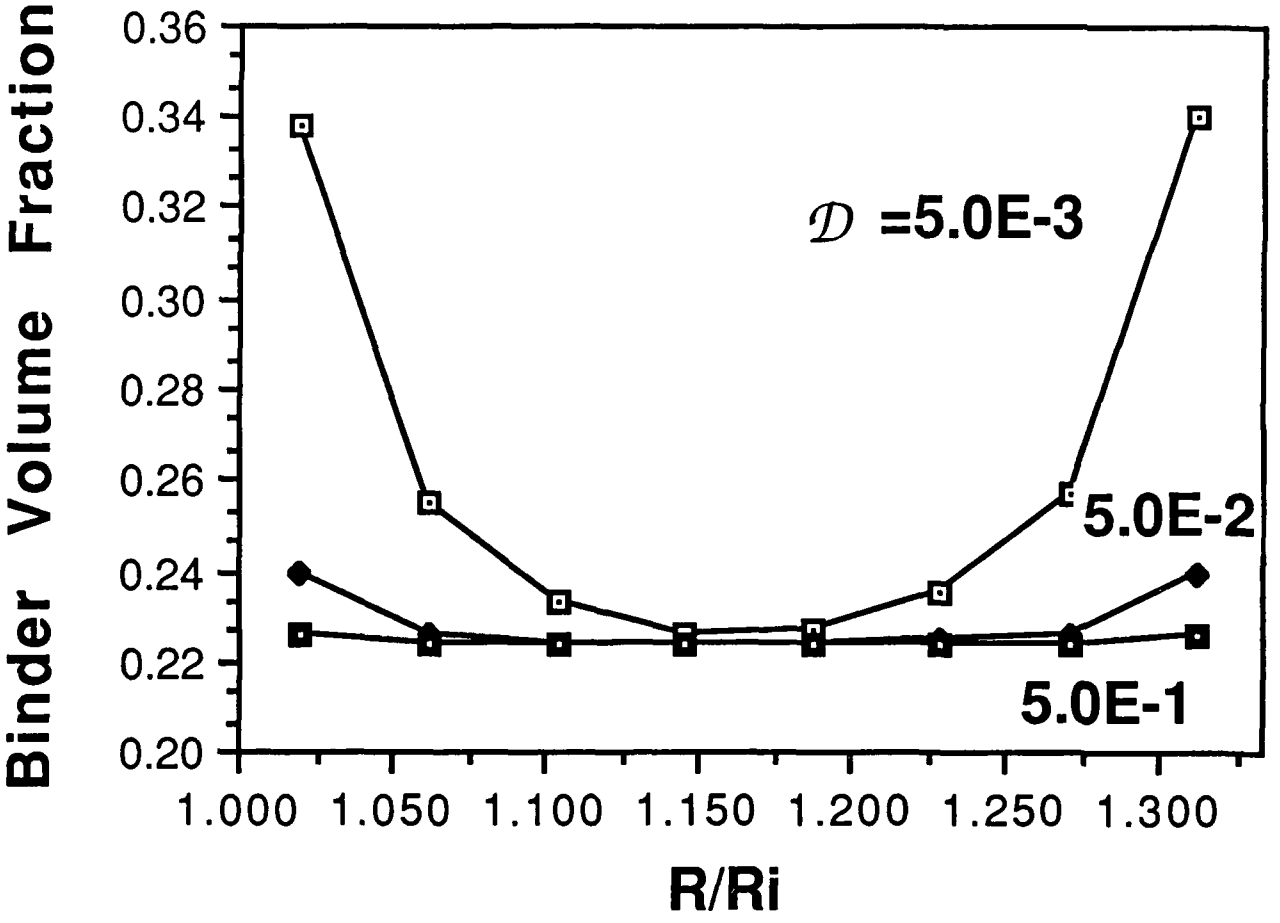

Fig. 3. Fully-Developed Binder Volume Fraction Distribution at the Exit of an Annular Duct (Z = 1)

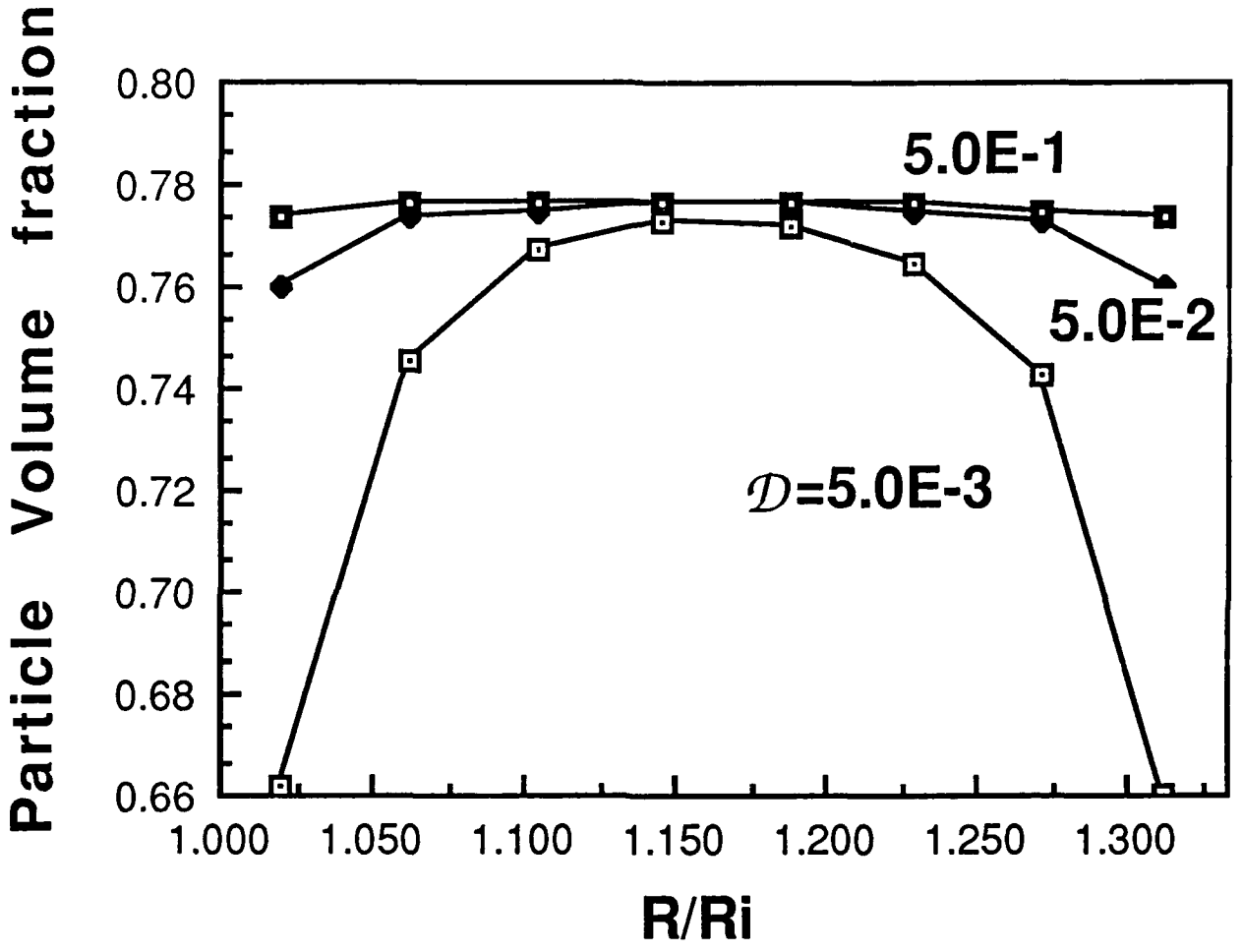

Fig. 4. Fully-Developed Particle Volume Fraction Distribution at the Exit of an Annular Duct (Z = 1)

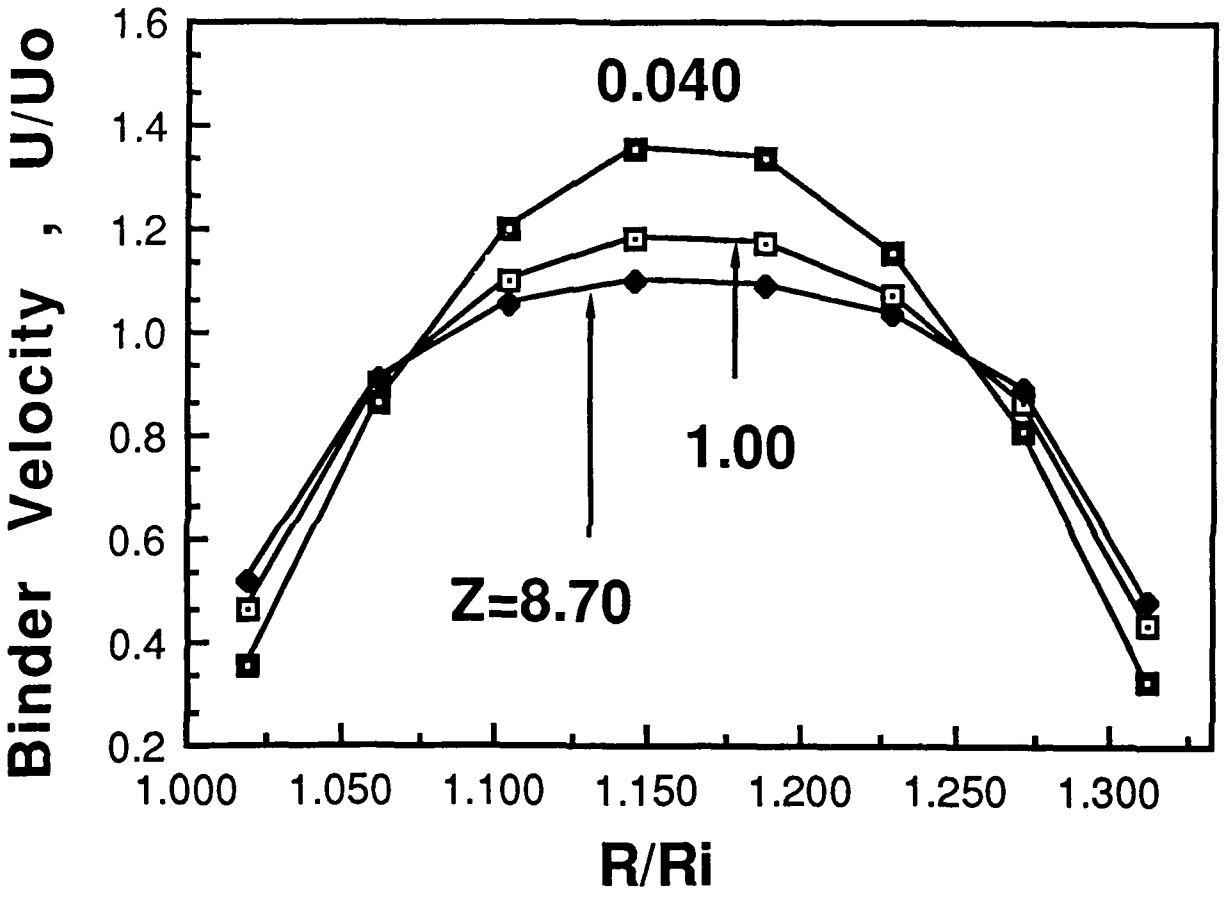

Fig. 5. Fully-Developed Binder Velocity Distribution at the Exit of an Annular Duct (D = 0.005)

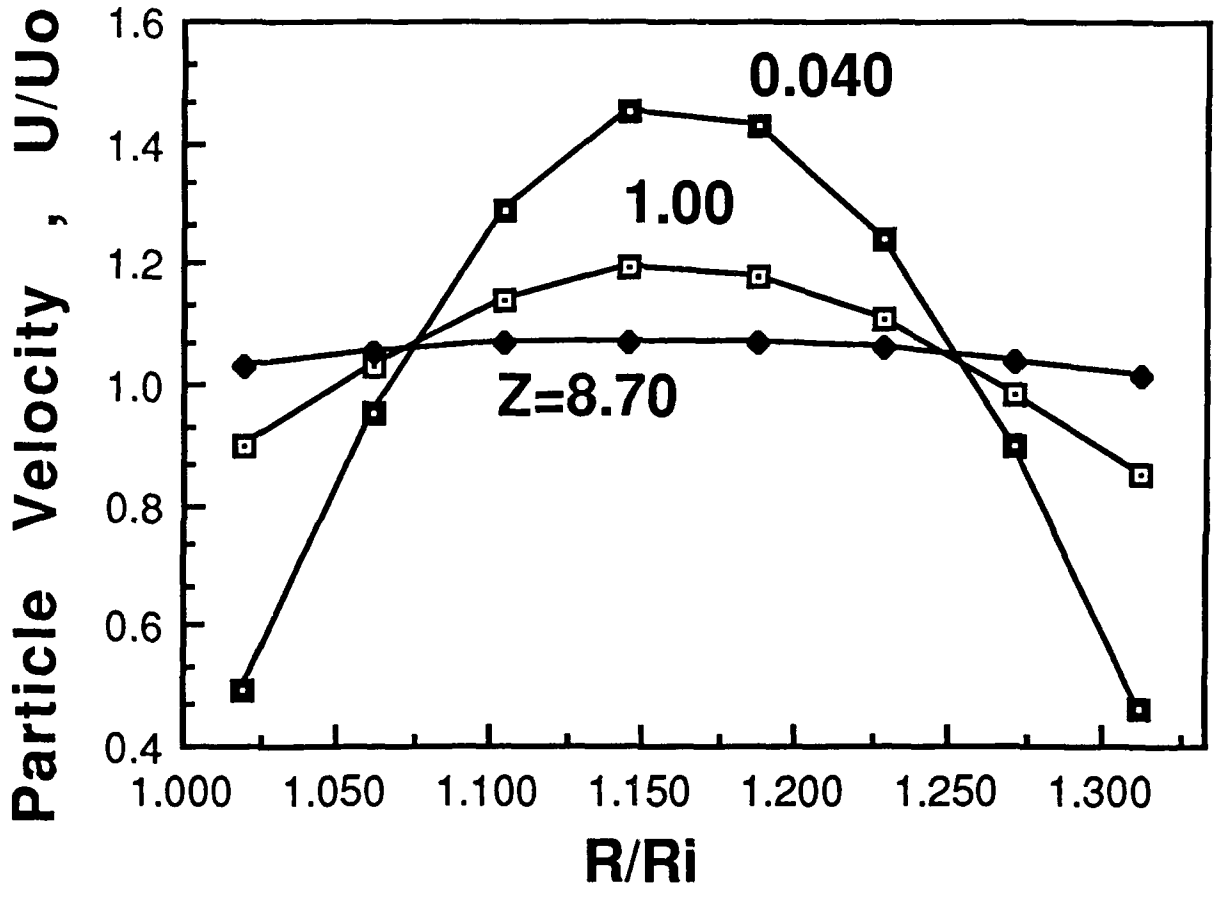

Fig. 6. Fully-Developed Particle Velocity Distribution at the Exit of an Annular Duct (D = 0.005)

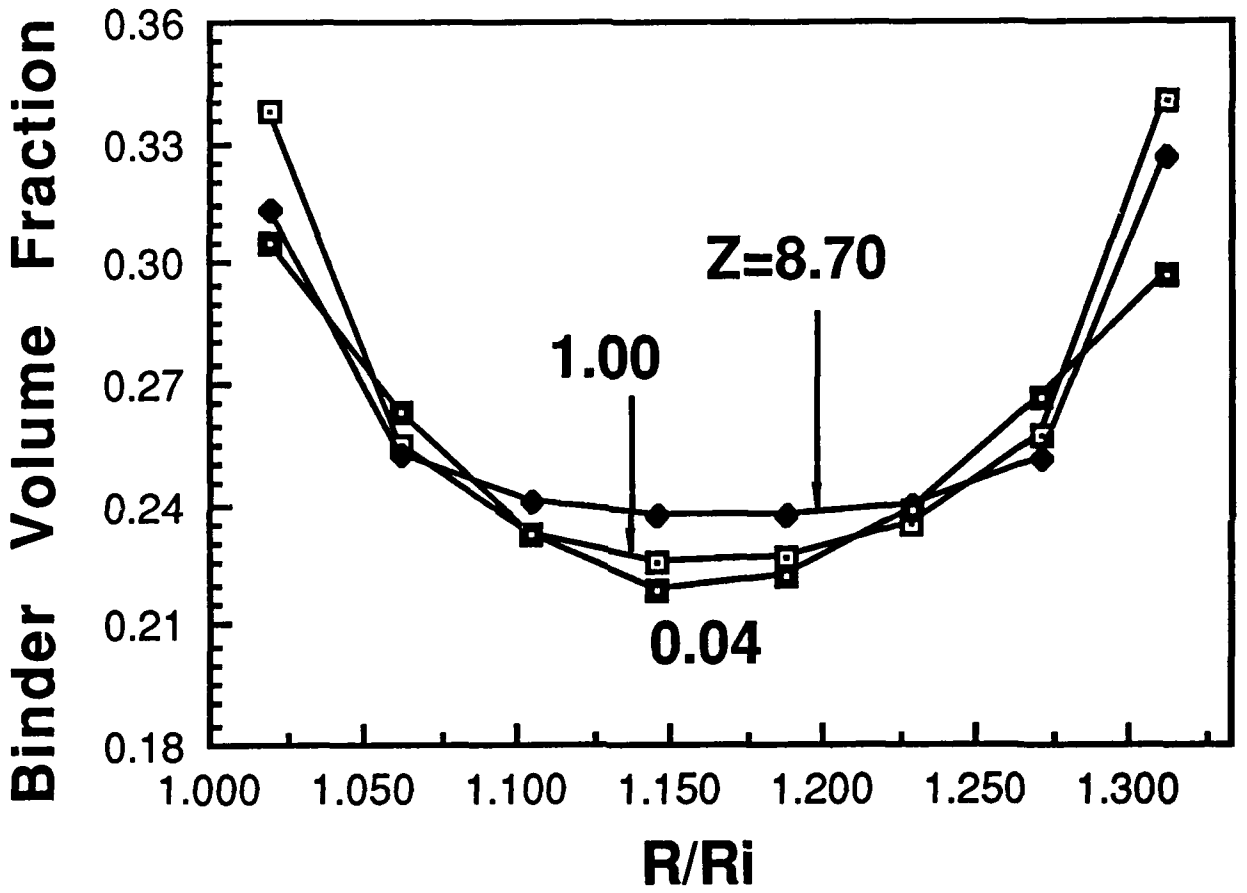

Fig. 7. Fully-Developed Binder Volume Fraction Distribution at the Exit of an Annular Duct (D = 0.005)

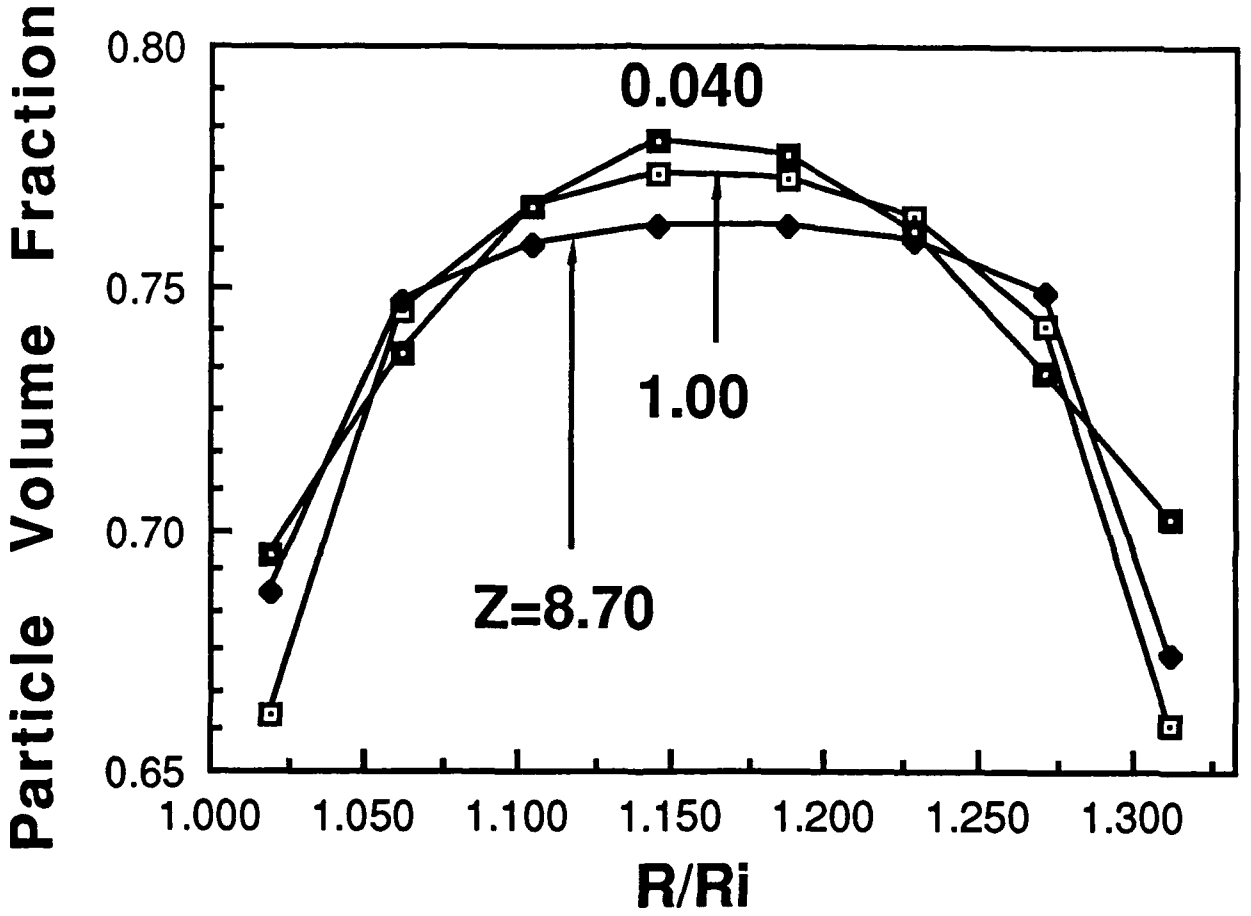

Fig. 8. Fully-Developed Particle Volume Fraction Distribution at the Exit of an Annular Duct (D = 0.005)

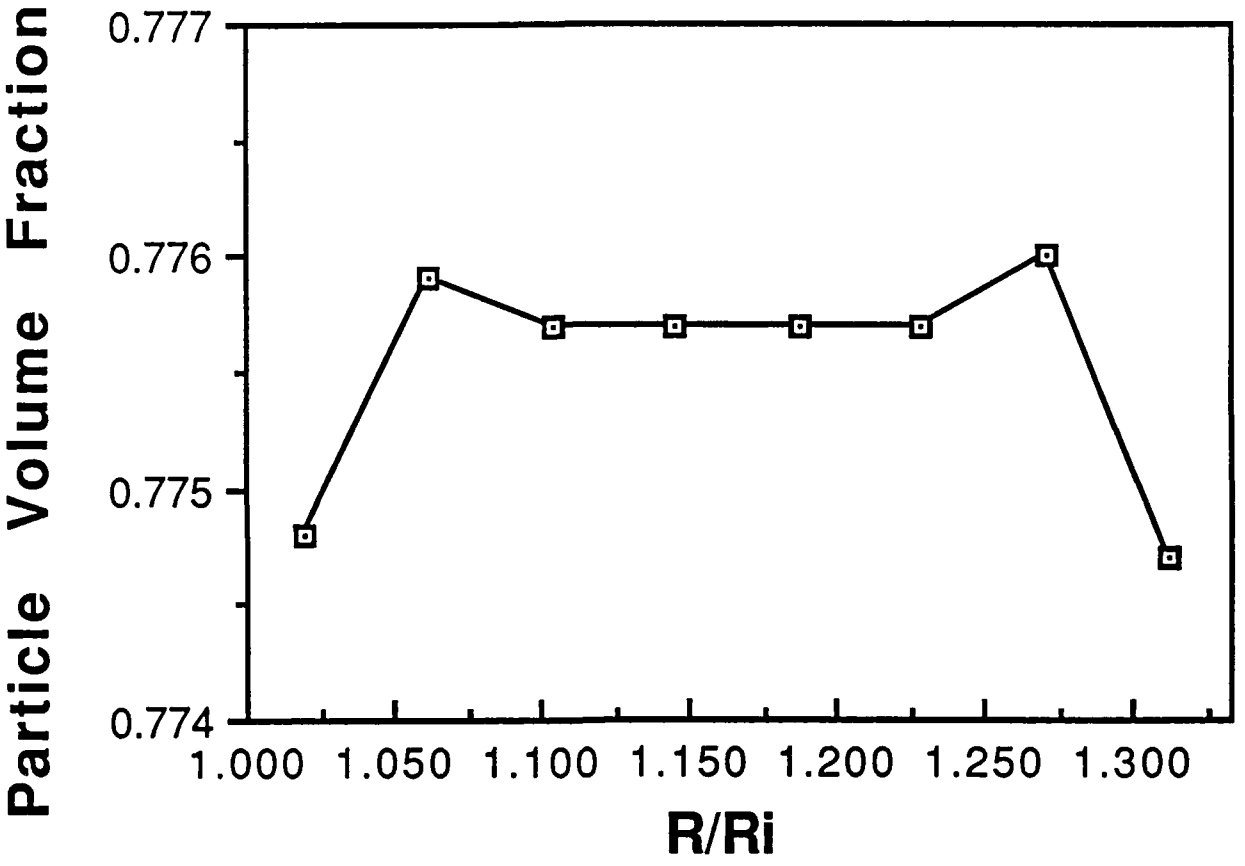

Fig. 9. Particle Volume Fraction Distribution at the Exit of an Annular Duct with D = 1 and Z = 10

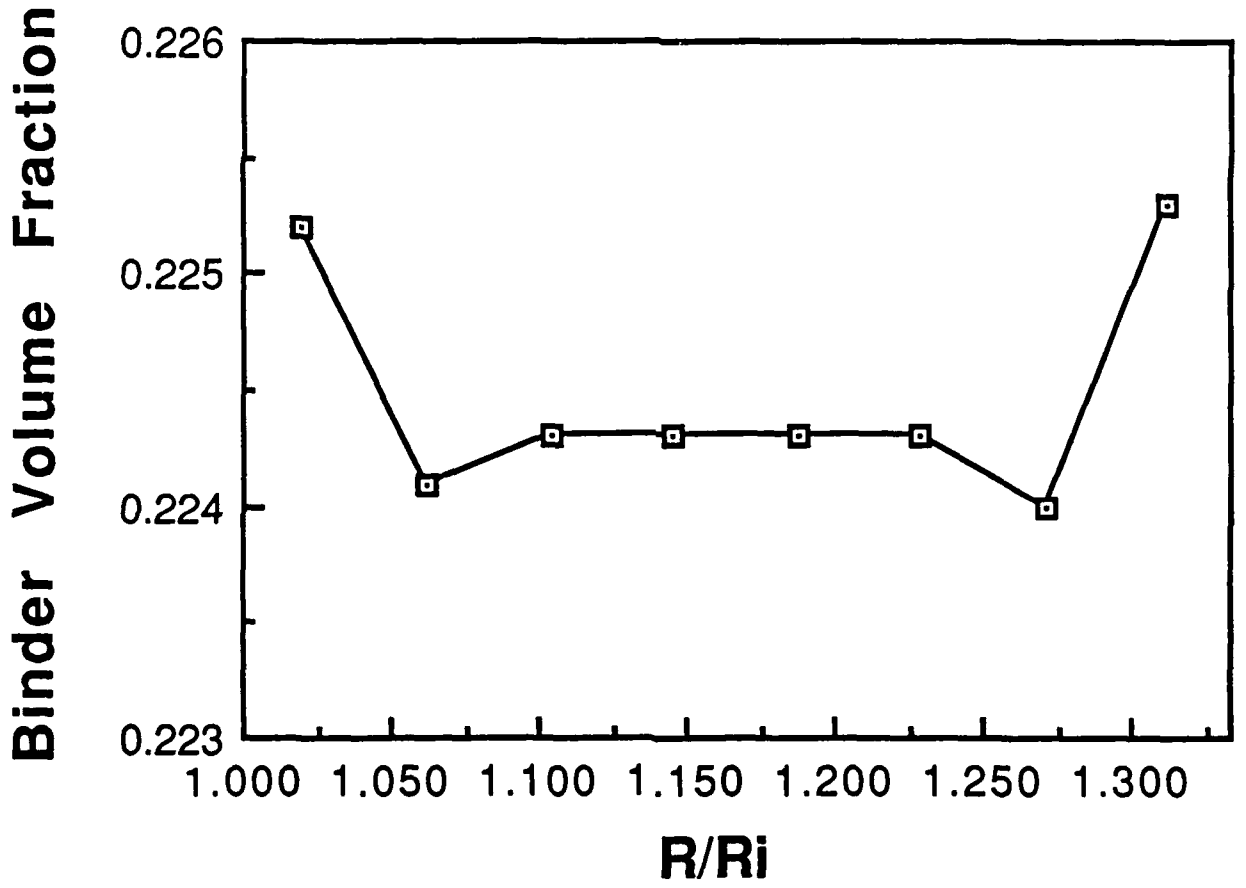

Fig. 10. Binder Volume Fraction Distribution at the Exit of an Annular Duct with D = 1 and Z = 10

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